Combinatorics and Arithmetic for Physics

Wave fronts with cross-diffusion

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November 7th, 2019

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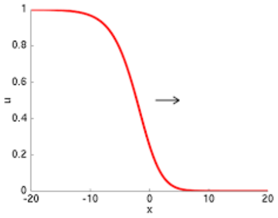
Existence of a travelling wave between the two states



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When $D_A = D_B$, the RD equation of $A(x,t)$ is a Fisher-KPP equation.

In a concentrated system, diffusion is perturbed:

$$\partial_t A = D_A \partial_x \left[\left(1 - \frac{A}{C} \right) \partial_x A \right] - D_B \partial_x \left(\frac{A}{C} \partial_x B \right) + kAB$$
$$\partial_t B = D_B \partial_x \left[\left(1 - \frac{B}{C} \right) \partial_x B \right] - D_A \partial_x \left(\frac{B}{C} \partial_x A \right) - kAB$$

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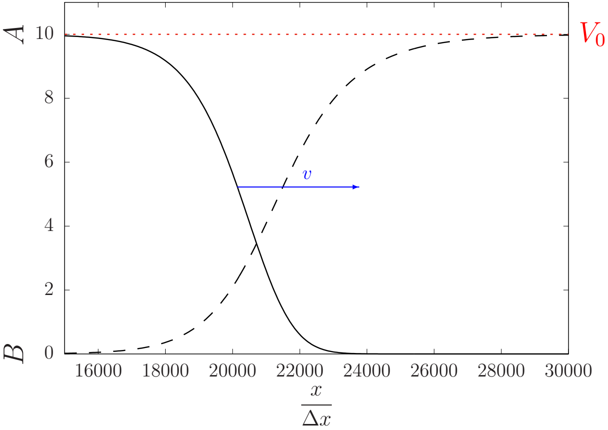
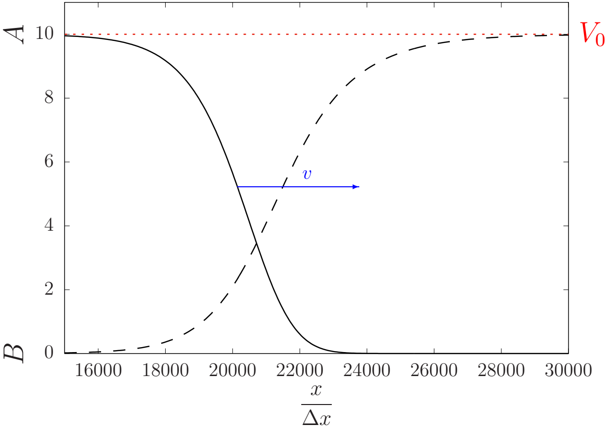
- **How does $D_A \neq D_B$ affect the velocity and shape of the wave front ?**
- **How does confinement (i.e. $S \to 0$) affect the velocity and shape of the wave front ?**
- **Can we use these effects to detect perturbed diffusion in a concentrated Fisher-KPP front ?**

Velocity v of a Fisher front



$$\boxed{v = 2\sqrt{kV_0 D_A}}$$

Velocity v of a Fisher front Independent of D_B and S



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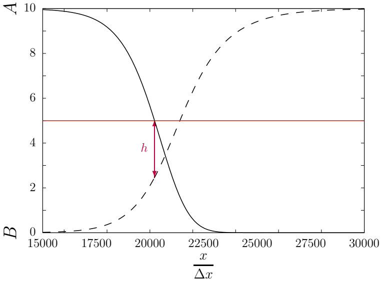
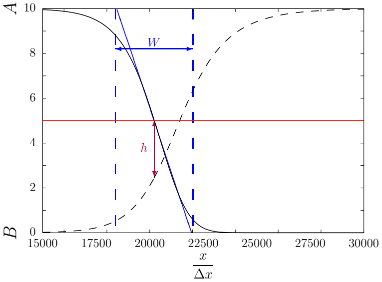
- **Height defined as the difference of concentration between $A(x_0)$ and $B(x_0)$ where $A(x_0) = \dfrac{V_0}{2}$**



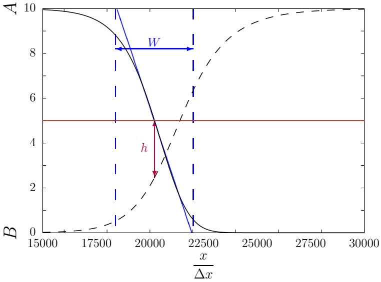
Shape of the front, 2 parameters:

- **Height** defined as the difference of concentration between $A(x_0)$ **and** $B(x_0)$ **where** $A(x_0) = \frac{V_0}{2}$
- **Width** of the front defined as the inverse of the slope of the A **profile where** $A(x_0) = \frac{V_0}{2}$



Shape of the front, 2 parameters:

- **Height** defined as the difference of concentration between $A(x_0)$ and $B(x_0)$ where $A(x_0) = \frac{V_0}{2}$ $\boxed{\Rightarrow h = B(x_0) - \frac{V_0}{2}}$
- **Width** of the front defined as the inverse of the slope of the A profile where $A(x_0) = \frac{V_0}{2}$ $\boxed{\Rightarrow W = \frac{V_0}{A'(x_0)}}$



To study the RD equations, we define the moving frame:

$$(x,t) \to (\zeta)$$
$$\zeta = \frac{x}{v} - t$$
$$\zeta_0 = \frac{x_0}{v} - t_0 \equiv 0$$
$$A(x,t) \to f(\zeta)$$
$$B(x,t) \to g(\zeta)$$
$$\epsilon = 1/v^2$$

$d =$ **dilute** (regular diffusion)

$c =$ **concentrated** (perturbed diffusion)

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Examples:

$f_d =$ **A concentration in the dilute case**

$g_c =$ **B concentration in the concentrated case**

Dilute case RD equations in the moving frame:

$$0 = k f_d g_d + f_d' + \epsilon D_A f_d''$$
$$0 = -k f_d g_d + g_d' + \epsilon D_B g_d''$$

Dilute case RD equations in the moving frame:

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\end{aligned}
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Concentrated case RD equations in the moving frame:

$$
0 = k f_c g_c + f_c' + \epsilon \left(D_A \left[\left(1 - \frac{f_c'}{C} \right) f_c'' - \frac{(f_c')^2}{C} \right] - D_B \left[\frac{f_c g_c''}{C} + \frac{f_c' g_c'}{C} \right] \right)
$$

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0 = -k f_c g_c + g_c' + \epsilon \left(D_B \left[\left(1 - \frac{g_c'}{C} \right) g_c'' - \frac{(g_c')^2}{C} \right] - D_A \left[\frac{g_c f_c''}{C} + \frac{f_c' g_c'}{C} \right] \right)
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We consider k, V_0 and D_A such as:

$$\epsilon \ll 1$$

Diffusion can be considered as a perturbation of reaction (do not mix up with perturbed diffusion !).
We write f and g as a perturbation series:

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + ...$$
$$g = g_0 + \epsilon g_1 + \epsilon^2 g_2 + ...$$

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Zero-th order solutions (no diffusion) are straightforwardly obtained:

$$f_{d,0} = f_{c,0} = \frac{V_0}{1 + e^{kV_0\zeta}}$$
$$g_{d,0} = g_{c,0} = \frac{V_0}{1 + e^{-kV_0\zeta}}$$

Now, instead of deriving the solutions for the higher-order terms $f_{1,2,\ldots}$ and $g_{1,2,\ldots}$, we focus on the point $\zeta_0 = 0$.

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The expressions for the height and the width, up to the second-order, are given by:

$$h_d = \frac{V_0}{16}\left(1-\frac{D_B}{D_A}\right)\left[1+\frac{1}{8}\left(1-\frac{D_B}{D_A}\right)\right]$$

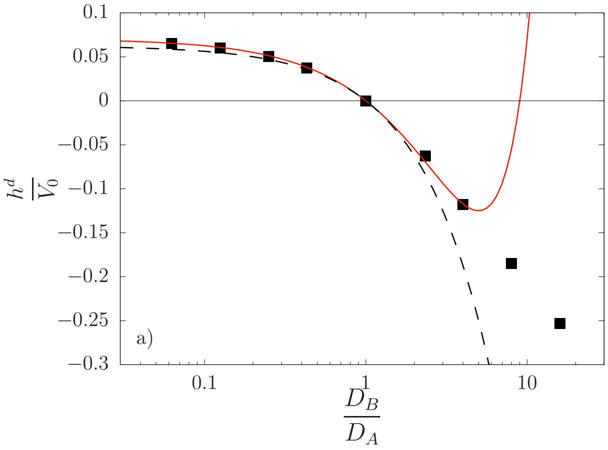
$$h_c = \frac{V_0}{16}\left(1-\frac{D_B}{D_A}\right)\left(1-\frac{V_0}{C}\right)\left[1+\frac{1}{8}\left(1-\frac{D_B}{D_A}\right)\left(1-2\frac{V_0}{C}\right)\right]$$

$$W_d = 8\sqrt{\frac{D_A}{kV_0}}\left[1+\frac{1}{8}\left(1-\frac{D_B}{D_A}\right)-\frac{1}{64}\frac{D_B}{D_A}\left(3-\frac{D_B}{D_A}\right)\right]^{-1}$$

$$W_c = 8\sqrt{\frac{D_A}{kV_0}}\left[1+\frac{1}{8}\left(1-\frac{D_B}{D_A}\right)\left(1-\frac{3V_0}{2C}\right)-\frac{1}{64}\left[\frac{D_B}{D_A}\left(3-\frac{D_B}{D_A}\right)\right.\right.$$
$$\left.\left.+\left(\frac{9}{2}-8\frac{D_B}{D_A}+\frac{7}{2}\frac{D_B^2}{D_A^2}\right)\frac{V_0}{C}-\left(\frac{7}{2}-7\frac{D_B}{D_A}+\frac{7}{2}\frac{D_B^2}{D_A^2}\right)\frac{V_0^2}{C^2}\right]\right]^{-1}$$

Comparison between analytic and numerical results:

Comparison between analytic and numerical results: Height in the diluted case



Perturbed diffusion ($V_0/C = 0.25$) vs. regular diffusion ($V_0/C = 0$):

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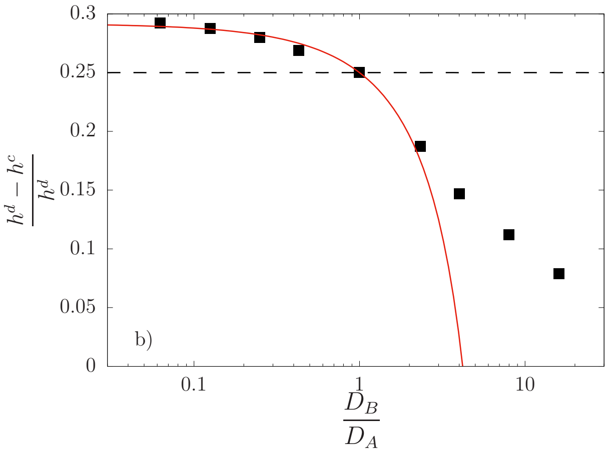

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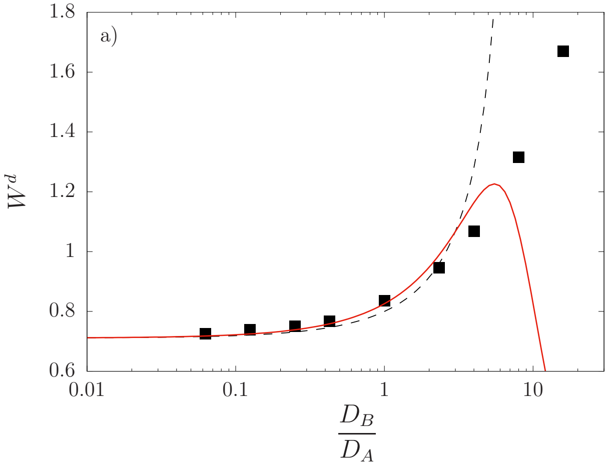

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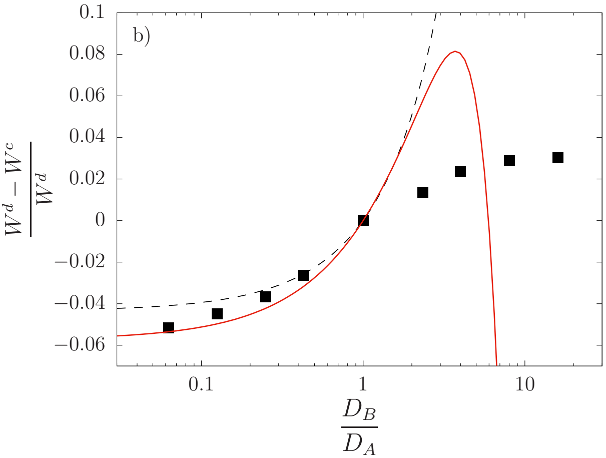

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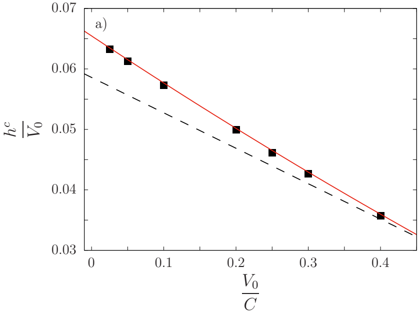
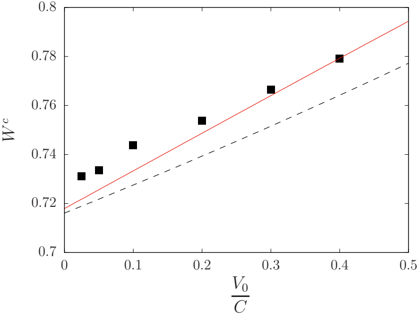


Width



for $D_B/D_A = 1/16$

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- **The shape of the front is affected by both effects. The height is strongly influenced by the ratio of diffusion coefficients D_B/D_A and the deviation from ideal solution V_0/C. However, its discriminating property is more efficient for low values of D_B/D_A.**
- **The width is also mainly affected by the ratio D_B/D_A and V_0/C, working better for large values of D_B/D_A.**

Thank You

[1] Morgado, Nowakowski, Lemarchand, Phys. Rev. E **99**, 022205 (2019)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 711859.

Cross-diffusion terms derivation from linear irreversible thermodynamics

The entropy production per unit mass due to isothermal diffusion is given by:

$$\sigma = \frac{1}{T} \sum_{X=A,B,S} \vec{\jmath}_X \cdot \left(-\vec{\nabla} \mu_X \right)$$

where T is the temperature, $\vec{\jmath}_X$ the flux of species X, and μ_X is the chemical potential of species X.
We consider the framework of the solvent. The flux of species X in this framework is defined by:

$$\begin{aligned} \vec{\jmath}^{\,*}_X &= \rho_X \left(\vec{u}_X - \vec{u}_S \right) = \rho_X \left(\vec{u}_X - \vec{u} \right) + \rho_X \left(\vec{u} - \vec{u}_S \right) \\ &= \vec{\jmath}_X - \frac{\rho_X}{\rho_S} \vec{\jmath}_S \end{aligned}$$

where ρ_X is the concentration of X, and $\vec{u}_X$ is the velocity of X.

Prigogine's theorem: **Entropy production does not depend on the chosen framework.**

Therefore:

$$\sigma = \frac{1}{T} \sum_{X=A,B,S} \vec{\jmath}_X \cdot \left(-\vec{\nabla}\mu_X\right) = \frac{1}{T} \sum_{X=A,B} \vec{\jmath}^{\,*}_X \cdot \left(-\vec{\nabla}\mu_X\right)$$

Assuming that the solution is ideal, we can write:

$$\mu_X = \mu_X^0 + RT \ln \frac{\rho_X}{\rho}$$

Using the expression for $\vec{\jmath}^{\,*}_X$ and μ_X, we get:

$$\begin{pmatrix} \vec{\jmath}_A \\ \vec{\jmath}_B \end{pmatrix} = \begin{pmatrix} 1 - \frac{\rho_A}{\rho} & -\frac{\rho_A}{\rho} \\ -\frac{\rho_B}{\rho} & 1 - \frac{\rho_B}{\rho} \end{pmatrix} \begin{pmatrix} \vec{\jmath}^{\,*}_A \\ \vec{\jmath}^{\,*}_B \end{pmatrix}$$

Using the expression for $\vec{j}^*_X$ and μ_X, we get:

$$\begin{pmatrix} \vec{j}_A \\ \vec{j}_B \end{pmatrix} = \begin{pmatrix} 1 - \dfrac{\rho_A}{\rho} & -\dfrac{\rho_A}{\rho} \\ -\dfrac{\rho_B}{\rho} & 1 - \dfrac{\rho_B}{\rho} \end{pmatrix} \begin{pmatrix} \vec{j}^*_A \\ \vec{j}^*_B \end{pmatrix}$$

Hypothesis: $\vec{j}^*_X = -D_X \vec{\nabla} \rho_X$ **(Fick's first law in solvent framework)**

Then:

$$\begin{pmatrix} \vec{j}_A \\ \vec{j}_B \end{pmatrix} = - \begin{pmatrix} 1 - \dfrac{\rho_A}{\rho} & \dfrac{\rho_A}{\rho} \\ \dfrac{\rho_B}{\rho} & 1 - \dfrac{\rho_B}{\rho} \end{pmatrix} \begin{pmatrix} D_A \vec{\nabla} \rho_A \\ D_B \vec{\nabla} \rho_B \end{pmatrix}$$